

Tetradecane  
629-59-4 | DTXSID1027267

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.14e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.25e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tridecane</div> <div>Measured: 1.16e-02</div> <div>Predicted: 6.33e-02</div>	<div>Image not found</div> <div>Octane, 1-iodo-</div> <div>Measured: 5.58e-02</div> <div>Predicted: 1.82e-01</div>	<div>Image not found</div> <div>Tetradecane</div> <div>Measured: 3.43e-03</div> <div>Predicted: 1.14e-02</div>
<div>Image not found</div> <div>Dialifor</div> <div>Measured: 4.54e-03</div> <div>Predicted: 1.07e-07</div>		